2664-Pos Board B650
Study of Cholesterol-Diacylglycerol-Pc Interactions in POPC Bilayer using Molecular Dynamics Simulation
Mohammad Alwarawrah, Jian Dai, Juyang Huang.
Diacylglycerol(DAG)-cholesterol-phospholipid interactions have received increasing attention for their involvement in lipid rafts. The interaction of DAG with *1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine* (POPC) and cholesterol were systematically investigated via atomistic molecular dynamics (MD) simulation. Four independent bilayer simulations (i.e., pure POPC, POPC/Cholesterol, POPC/DAG, and POPC/DAG/Cholesterol) were performed at 310K. Cholesterol and DAG both have small hydrophilic headgroups and large hydrophobic bodies. The 2D radial distribution functions of molecules show an Umbrella effect between cholesterol and POPC, and also between DAG and POPC. In the ternary mixture of POPC/DAG/cholesterol, cholesterol increases the order parameters of POPC acyl chains as well as DAG acyl chains. The average distances between acyl chains of POPC and DAG decrease with the addition of cholesterol. The cholesterol tilt angle with the bilayer normal in POPC/DAG/cholesterol bilayer is smaller than that in POPC/cholesterol bilayer.

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Inter-Leaflet Interaction and Asymmetry in Phase Separated Lipid Bilayers: Molecular Dynamics Simulations
Jason D. Perlmutter, Jonathan N. Sachs.
In order to investigate experimentally inaccessible, molecular-level detail regarding inter-leaflet interaction in model membranes, we have run an extensive series of coarse-grained molecular dynamics simulations of phase-separated lipid bilayers, totaling over 150 microseconds. This has allowed us to investigate three types of inter-leaflet coupling within a bilayer: 1) The effect of phase asymmetry on lipid structure and dynamics; 2) the effect of phase asymmetry on local curvature; and 3) spatial registration of domains in compositionally symmetric bilayers. In particular, we show that phase asymmetry leads to changes in acyl chain tilt, lipid rotational dynamics and lateral diffusion. Secondly, in phase asymmetric bilayers, phase separated leaflets resist curvature, while inducing curvature in an opposing disordered leaflet. And, third, in bilayers containing compositional symmetry, the registration of domains in opposing leaflets depends upon acyl chain length: registration vs. anti-registration appears to be dictated by the energetic cost of a height mismatch between neighboring phases.

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A coarse-Grained Solvent-Free Model for Tethered Lipid Membrane Simulation
Mingyang Hu, Markus Deserno.
In order to characterize biological lipid membranes and their constituents, a variety of experimental techniques, for instance fluorescence microscopy and X-ray/neutron reflection, require the bilayer systems to have a robust planar geometry. However, the adsorption onto a substrate can strongly affect some properties of the system, especially in the proximal leaflet. To alleviate artifacts such as the immobility of membrane-associated proteins, tethered bilayer systems have been developed. In these systems tethers consisting of short hydrophilic polymers elevate the bilayer from the substrate and also provide better control over the separation between the two.
Different computational models for lipid memebranes with varying levels of resolution have been proposed in the past. However, only a few simulations have been dedicated to the supported systems, and none have studied the tethered bilayers. Here we present a mesoscopic coarse-grained model of tethered lipid membranes, which is based on an implicit-solvent three-bead lipid model [Cooke et. al., Phys. Rev. E 72, 011506 (2005)]. Each tether molecule consists of 1) a hydrophobic part that can anchor into lipid leaflets and share the properties of the lipids, 2) a hydrophilic chain mimicking polyethelene glycol, and 3) a headgroup bead which covalently attaches to the substrate. Under suitable conditions, these fixed tether molecules and free random lipids self-assemble into a flat tethered bilayer. Different physical observables, such as the fluctuation spectrum, the area density of lipids, and diffusion coefficients in proximal/distal leaflets, are measured. The results are compared to free and solid-supported membranes, providing important insights into the generic properties of this system.

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Studies of Phase Transition(s) in Phospholipid/Cholesterol Systems by Molecular Dynamics Simulations
Qaiser Waheed, Olle Edholm.
Molecular dynamics simulations of atomistic models show the ordering and condensing effect of the cholesterol on phospholipid bilayers. Such simulations are, however, too time consuming to permit monitoring of the gel/liquid crystalline phase transition. We used therefore the simplified coarse grained MARTINI model to study the phase transition in dipalmitoylphosphatidylcholine (DPPC) cholesterol mixtures. A recent study by Marrink shows that this model is able to describe the main phase transition of pure phospholipid systems reasonably.
The area per molecule was calculated separately for the phospholipids and cholesterol as a partial specific area (Edholm & Nagle). The condensation effect of cholesterol is obtained with the atomistic model as a negative partial specific area for cholesterol. The coarse grained model reproduce the condensation effect and gives a negative partial specific area of cholesterol molecule at low cholesterol concentration and low temperatures above the main phase transition. The main phase transition occurs already at about 295K for the coarse grained model. There is, however, another (second order) phase transition at 304K, where partial specific area suddenly becomes positive for all cholesterol concentrations. Such a transition was, however, not observed with the atomistic model. A similar transition was observed in the order parameter versus temperature at low cholesterol concentration, but this vanishes at high concentration. These results were used to test different suggested relations between area per lipid and the order parameter. Below, the main transition, the radial distribution functions and chain order parameters were used to monitor the difference between long range positional order and chain order as well as to search for inhomogeneities in the lipid distribution.

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Determination of the Gaussian (Saddle-Splay) Modulus for Lipid Bilayers from Atomistic and Coarse Grained Simulations
Olle Edholm, Erik G. Brandt.
The bending modulus of lipid bilayers is easily determined from the Fourier transform of the undulation intensity from molecular dynamics simulations. In several studies during the last ten years this has been found in good agreement with experiment. The saddle splay modulus is more difficult to determine experimentally, but most experiments indicate that it is negative and has a magnitude of about half that of the bending modulus. Simulations are usually done with periodic boundary conditions which gives a system with zero mean Gaussian curvature due do Gauss-Bonnets theorem. Therefore, the saddle splay modulus could not be inferred from from intensities in Fourier space. We show here that values may be obtained by calculating the Gaussian curvature in real space at different points from splined snapshots of membrane surfaces.

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Direct Fourier Analysis of Lipid Bilayer Fluctuations in Particle-Based Simulations
Erik G. Brandt, Anthony R. Braun, Jonathan N. Sachs, John F. Nagle, Olle Edholm.
The particles in the lipid bilayer undergo fluctuations from their equilibrium positions. These motions are best described in terms of correlated monolayer motions (undulations), anticorrelated monolayer motions (thickness fluctuations) and number density correlations, both within and between the monolayers. Particle-based computer simulations, atomistic or coarse-grained, can be used to calculate the spectra of these equilibrium fluctuations. This has conventionally been done by interpolating the particle structure onto a grid to facilitate for the discrete Fourier transform. However, the gridding introduces artifacts and an upper cutoff on the available wave vectors.
Here, we instead analyze the simulations directly in Fourier space, circumventing the need for a grid approximation. The fluctuation spectra can then be calculated at high precision up to any wave vector desired, and the low wave vectors are only bounded by the size of the lateral simulation box. From the analysis, a picture emerges which bridges a continuum regime at low wave vectors, and a domain that can be attributed to the in-plane bilayer molecular structure at high wave vectors. We calculate spectra for undulations, thickness fluctuations, and the spectrum of the number density along the undulating surface, and we discuss how the shape of the spectra in the low-wave vector and high-wave vector regimes are related to membrane material constants, and give some predictions from an analytical theory based on equilibrium correlation functions.

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The Elastic Properties of Membranes Adhering to Solid Surfaces
Max C. Watson, Frank L.H. Brown, Paul Welch.
Lipid bilayers are frequently studied on top of solid substrates and recently, their behavior in contact with spherical particles has attracted considerable attention. Though many techniques are available for finding the material properties of freely suspended membranes, determining the elastic moduli of a membrane bound to a solid surface has not yet been possible. Using coarse-grained molecular dynamics simulations, we demonstrate how these properties are in fact accessible by analyzing the thermal fluctuations of the individual lipids.